Vitinoin

Inchi: InChI=1S/C20H28O2/c1-15(8-6-9-16(2)14-19(21)22)11-12-18-17(3)10-7-13-20(18,4)5/h6
InchiKey: SHGAZHPCJJPHSC-UHFFFAOYSA-N
Formula: C20H28O2
SMILES: CC(C=CC1=C(C)CCCC1(C)C)=CC=CC(C)=CC(=O)O
Mol. weight [g/mol]: 300.44
CAS: 302-79-4

Physical Properties

Property code	Value	Unit	Source
hfus	41.87	kJ/mol	Joback Method
ie	7.68	eV	Cheméo Relay (1.0)
logp	5.603		Crippen Method
mcvol	267.740	ml/mol	McGowan Method
tf	454.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.46020e+02
Coeff. B	2.27350e+00
Coeff. C	-1.94340e-03
Coeff. D	7.10000e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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